Preface

Due to their diversity, soft matter systems provide a convenient platform to study a variety of physical phenomena like phase transitions and collective motion. Encompassing a wide range of equilibrium and non-equilibrium systems, they often provide significant insight into the statistical mechanics of different kinds of many-body systems. Though large scale properties of such systems are of fundamental interest in their own accord, since most experimental realizations of soft matter systems are finite sized, there is a growing need to understand the effects of confinement or boundary conditions on the collective behaviour of such systems. The primary purpose of this thesis is to study the effects of boundary conditions or confinement on both equilibrium and non-equilibrium soft matter systems via theoretical modelling. For equilibrium systems we have studied a system of colloidal particles in harmonic confinement, and for non-equilibrium systems we consider a system of self-propelled rods in both harmonic and hard wall confinement.

In **Chapter 1** we first lay down some basic concepts of stochastic dynamics and Brownian motion, before discussing some of the recent results on confinement effects on colloidal systems, showing how the properties of a finite sized colloidal system can be very different from those of large, unconfined systems. Thereafter turning to non-equilibrium active systems, we discuss various fundamental problems posed by these systems due to their unique ability to generate and dissipate energy on their own. We also point out some instances of observed confinement effects in such systems, such as boundary aggregation and transient hedgehog-like clusters near the boundary.

Chapter 2 deals with the effect of harmonic confinement on a finite sized colloidal assembly, where we show that such finite size effects coupled with a confining potential can give rise to special features like initial position dependent expulsion of dopant particles. First we model experimentally studied small two-dimensional colloidal assemblies trapped by a defocussed laser beam by Langevin dynamics simulations in the presence of harmonic confinement and demonstrate how the system shows a crossover from liquid state to crystalline state as a function of the stiffness of the confinement. We also show that in the crystalline state the system can be effectively modelled as a rigid body under small force perturbations. Notably, while studying the dynamics of a defect particle inside these crystallites, we found evidence for the occurrence of self purification by the crystallites. In this process, a dopant is spontaneously expelled out of the crystallite. Surprisingly, this phenomena has a strong dependence on the initial position of the dopant, which turns out to be the consequence of the non monotonic spatial variation of the free energy of the system as a function of the dopant position. This is caused by a difference in the rate of change of internal energy and entropy with the dopant position, with the entropy decreasing faster when the dopant is closer to the centre. This can be attributed to the amount of disruption of crystalline order in the assembly due to the incommensurate dimensions of the defect particle. In order to put these results in a general perspective, we verify in the last part of this chapter that the presence of this free energy barrier is independent of the exact functional forms of the confining potential and the interaction of a defect particle with the host particles, as well as the shape and size of the defect particle.

Moving to non-equilibrium systems, we consider, in **Chapter 3**, the effect of harmonic and hard wall confinement on a two-dimensional system of self-propelled rods (SPRs). Though there have been very limited studies of confinement effects on such systems, existing studies are adequate to show that their behaviour near a boundary wall can be very different, *e.g.* formation of hedgehog like clusters near a boundary wall. First we show that for harmonic confinement small systems show polar order, which decays with system size, eventually going away for large systems. But the effect of hard wall confinement turns out to be rather different, where the system shows isotropic and clustered states depending on the values of activity and density. We construct a complete activity-density phase diagram showing four distinct phases. For high density and high activity, the rods spontaneously arrange themselves into a stable vortex structure in which the rods exhibit global radial polar order. Surprisingly this order does not decay with system size: the radial orientation of the rods exhibit strong spatial correlation even in large systems, ruling out the possibility that the radial order is a finite-size effect. Using other geometrical shapes of the hard wall boundary, we confirm this phase to be independent of the shape of the boundary. We also demonstrate how small modifications of the boundary conditions at the hard wall can collapse the clustered and vortex phases to a global flocking phase similar to that found in earlier studies of hydrodynamic active particles under confinement. Based on these observations, we conclude that the bulk of the system is strongly affected by the subjected boundary condition, which is rather unusual for large systems.

In **Chapter 4** this thesis concludes with a summary of the main results and suggestions for future work along similar lines.